The gradient flow running coupling scheme

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The Yang-Mills gradient flow in finite volume is used to define a running coupling scheme. As our main result the discrete β-function, or step scaling function, is calculated for scale change $s = 3/2$ at several lattice spacings for $SU(3)$ gauge theory coupled to $N_f = 4$ fundamental massless fermions. The continuum extrapolation is performed and agreement is found with the continuum perturbative results for small renormalized coupling. The case of $SU(2)$ gauge group is briefly commented on.

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1. Introduction

The Yang-Mills gradient flow is a relatively new addition to the arsenal of non-perturbative tools for the study of non-abelian gauge theories [1, 2, 3]; see also [4, 5] for its use in a slightly different context. It has been usefully implemented for a high precision scale determination in QCD [6] as well as for a running coupling scheme in a finite volume setup [7], among others.

All these applications involve the operator $\text{Tr}F_{\mu\nu}F_{\mu\nu}$ and its derivative with respect to the gauge field. The discretized expression of the derivative is then used in a finite step integration scheme of the gradient flow,

$$\frac{dA_\mu(t)}{dt} = -\frac{dS_{YM}(A)}{dA_\mu} \,.$$ (1.1)

The operator $\text{Tr}F_{\mu\nu}F_{\mu\nu}$ enters the simulations at two other instances. First, it is simply used in the gauge action for generating the configurations and second in the observable
$\langle E(t)\rangle = -\frac{1}{2}\langle \text{Tr}F_{\mu\nu}(t)F_{\mu\nu}(t)\rangle$ i.e. the field strength tensor squared evaluated at flow time $t > 0$. For the gauge action we use the tree level Symanzik improved action and for $E(t)$ the same clover improved discretization is employed as in [1, 6, 7]. For the derivative along the flow (1.1) we have used both the Wilson discretization and the tree level Symanzik variant but found that the scaling properties of the latter are more favorable for our present investigation and hence will only use that one.

Our goal is to compute the running coupling in $SU(3)$ gauge theory coupled to $N_f = 4$ flavors of massless fundamental fermions. The main observable is the discrete β-function in a finite volume setup where the running is with the linear size of the system, similarly to the Schroedinger functional [8] and to other finite volume approaches. The discrete β-function corresponding to a scale change of s is $(g^2(sL) - g^2(L))/\log(s^2)$, where the renormalized coupling $g^2(L)$ is obtained from the gradient flow.

The Schroedinger functional analysis of the same model, 4-flavor QCD, can be found in [9, 10].

2. Gradient flow scheme

The gradient flow (1.1) is used to define a renormalized coupling in finite volume by first fixing the ratio $\sqrt{8t}/L = c$ and then setting

$$g_c^2 = \frac{128\pi^2\langle t^2 E(t)\rangle}{3(N^2-1)(1+\delta(c))} \,,$$ (2.1)

where

$$\delta(c) = -\frac{c^4\pi^2}{3} + \vartheta^4\left(e^{-1/c^2}\right) - 1$$ (2.2)

is given in terms of the Jacobi elliptic function $\vartheta(q) = \sum_n q^{n^2}$. The numerical factors on the right hand side of (2.1) are such that to leading order $g_{\overline{\text{MS}}}^2 = g_c^2$ [7]. Corrections contain both even and odd powers of $g_{\overline{\text{MS}}}$. Different choices for the constant c correspond to different schemes but the

leading order relationship $g_{\overline{\mathrm{MS}}}^2 = g_c^2$ ensures that the 1-loop β-function in the gradient flow scheme coincides with the 1-loop β-function in the $\overline{\mathrm{MS}}$ scheme. The 2-loop β-function of the $\overline{\mathrm{MS}}$ scheme is on the other hand not the same as in the gradient flow scheme because of the non-zero a_1 term: $g_c^2 = g_{\overline{\mathrm{MS}}}^2(1 + a_1(c)g_{\overline{\mathrm{MS}}} + O(g_{\overline{\mathrm{MS}}}^2))$; for more details see [7].

Massless fermions can also be included if anti-periodic boundary conditions are used. The non-trivial boundary conditions cause the fermions to have an effective energy gap of order $1/L$ in small volume hence as one follows the running of the coupling from the UV towards the IR at least for small renormalized coupling the simulation will not run into problems even at zero bare fermion mass.

3. A note on the $SU(2)$ case

One might worry that for gauge group $SU(2)$ the matrix integrals in [7] used for the definition of the running coupling are not finite in $D = 4$ dimensions. The matrix integrals needed at leading order are

$$I_{D,N} = -\frac{\int dB \frac{1}{2}\mathrm{Tr}[B_\mu, B_\nu]^2 \exp\left(\frac{1}{2}\mathrm{Tr}[B_\mu, B_\nu]^2\right)}{\int dB \exp\left(\frac{1}{2}\mathrm{Tr}[B_\mu, B_\nu]^2\right)} \,, \tag{3.1}$$

where the integral dB is over D anti-hermitian traceless $N \times N$ matrices. Throughout this section we set $L = 1$. Both the numerator and denominator are finite in $D = 4$ and $N > 2$; see [11].

Clearly, one may evaluate $I_{D,N}$ from the matrix model partition function

$$Z_{D,N}(b) = \int dB \exp\left(\frac{b}{2}\mathrm{Tr}[B_\mu, B_\nu]^2\right) \tag{3.2}$$

via its logarithmic derivative,

$$I_{D,N} = -\left.\frac{d\log Z_{D,N}(b)}{db}\right|_{b=1} \,, \tag{3.3}$$

provided $Z_{D,N}(b)$ and its derivative are finite. For $D = 4$ and $N > 2$ this is the case and one easily obtains $I_{4,N} = N^2 - 1$. For $D = 4$ and $N = 2$ however $Z_{4,2}(b)$ is divergent. But the partition function $Z_{D,2}(b)$ can be evaluated for $D > 4$ and is in fact finite [12],

$$Z_{D,2}(b) = \frac{1}{2}\left(\frac{2\pi^2}{b}\right)^{\frac{3D}{4}} \frac{\Gamma(D/4)\Gamma(D/4 - 1/2)\Gamma(D/4 - 1)}{\Gamma(D/2)\Gamma(D/2 - 1/2)\Gamma(D/2 - 1)} \,. \tag{3.4}$$

The divergence in $D = 4$ is coming from the pole of $\Gamma(D/4 - 1)$. The logarithmic derivative of the above expression for $D > 4$ then leads to

$$I_{D,2} = \frac{3D}{4} \,, \tag{3.5}$$

which agrees with the result $N^2 - 1$ for $N = 2$ if $D = 4$ is set at the end of the calculation. Since the perturbative calculation of $\langle t^2 E(t)\rangle$ is performed in dimensional regularization and $D = 4$ is only set at the very end, the above procedure is natural.

One needs to be very careful about corrections which are only logarithmically suppressed [1]. This question was first discussed in [13]. A toy model where the issue at hand can be illustrated is

$$Z(g^2) = \int dxdy e^{-x^2-y^2-\frac{x^2y^2}{g^2}} , \tag{3.6}$$

with the associated expectation value $\langle x^2y^2 \rangle$. Let us introduce $b = 1/g^2$, then

$$\langle x^2y^2 \rangle = -\frac{\frac{dZ(b)}{db}}{Z(b)} . \tag{3.7}$$

A key feature of the gauge theory case, a flat direction in the tree level potential, is shared by the above toy problem. The tree level potential is x^2y^2/g^2 and the "1-loop" potential $x^2 + y^2$ is subleading. For finite g both the partition function and the expectation value are finite but the $g \to 0$ limit is quite subtle.

Naively, in the $g \to 0$ limit the "1-loop" potential $x^2 + y^2$ can be dropped to leading order but then both the numerator and denominator in (3.7) are divergent, similarly to the $SU(2)$ gauge theory case.

One might nevertheless first drop the $x^2 + y^2$ potential and then rescale the variables by $x \to \sqrt{g}x$ and $y \to \sqrt{g}y$ in order to obtain

$$\langle x^2y^2 \rangle = g^2 \frac{\int dxdy x^2y^2 e^{-x^2y^2}}{\int dxdy e^{-x^2y^2}} + \dots \tag{3.8}$$

where again both the numerator and the denominator are divergent. But since now the potential is a homogeneous polynomial, the above ratio is naively $1/2$, leading to

$$\langle x^2y^2 \rangle = \frac{g^2}{2} + \dots , \tag{3.9}$$

as the naive form of the small-g behavior. However exact evaluation of the integrals for finite g leads to

$$\langle x^2y^2 \rangle = \frac{g^2(1+g^2)}{2} - \frac{g^4}{2} \frac{K_1(g^2/2)}{K_0(g^2/2)} , \tag{3.10}$$

using the Bessel K-functions. The small-g expansion of the above is

$$\langle x^2y^2 \rangle = \frac{g^2}{2} \left(1 + \frac{2}{\log(g^2/4) + \gamma_E} \right) + O(g^4) , \tag{3.11}$$

where γ_E is Euler's constant. The naively obtained leading order $g^2/2$ result is supplemented by only logarithmically suppressed $O(g^2/\log(g^2))$ corrections not only polynomial ones like $O(g^4)$.

Ref. [13] discusses the $SU(2)$ theory, for which a similar logarithmic correction is expected. Note that the coefficient of the logarithmic term for the SU(2) theory is at present unknown.

Since all matrix integrals to leading order for $N > 2$ are finite we do not expect such complications for $SU(3)$ which is our main application. In high orders of $g_{\overline{MS}}$ similar logarithmic corrections may enter but not to leading order which ensures that in the UV the 1-loop β-function is the same in our scheme as in every other scheme.

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[1]DN is grateful to Martin Luscher for an instructive discussion of this point.
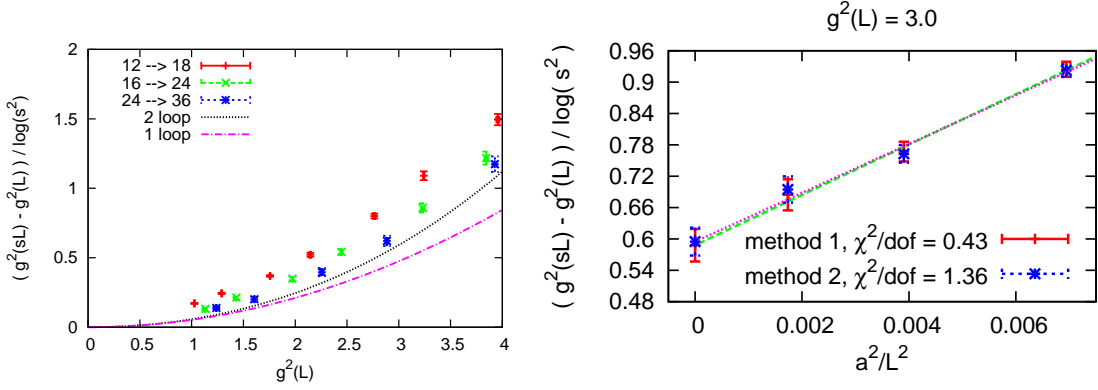
Figure 1: Discrete β-function of $SU(3)$ gauge theory coupled to $N_f = 4$ flavors of massless fundamental fermions. Left: scale change of $s = 3/2$, the results at 3 lattice spacings are shown together with the continuum universal 1-loop and $\overline{\text{MS}}$ 2-loop results for comparison. Right: continuum extrapolation of the discrete β-function for an illustrative value of the coupling $g^2(L) = 3$. Two methods were used to perform the continuum extrapolation; for details see [7]. The two methods give results which agree with each other for all of our $g^2(L)$ values.
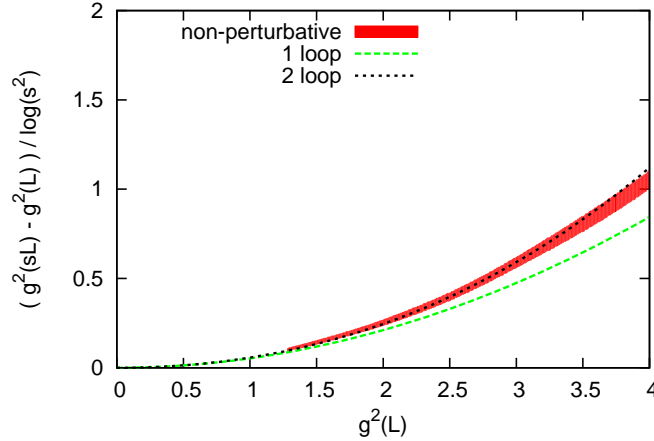
Figure 2: Discrete β-function of $SU(3)$ gauge theory coupled to $N_f = 4$ flavors of massless fundamental fermions for a scale change of $s = 3/2$. The continuum extrapolated result is shown together with the universal 1-loop and $\overline{\text{MS}}$ 2-loop results for comparison [7].

4. Results

Once the renormalized coupling is defined by (2.1) the discrete β-function, or step scaling function [14], can be computed by increasing the volume by a factor of s. The simulations were performed with the same parameters as reported in [7].

For the scale change $s = 3/2$ we have results for 4 lattice spacings, corresponding to the volume changes $8 \rightarrow 12$, $12 \rightarrow 18$, $16 \rightarrow 24$ and $24 \rightarrow 36$. The coarse lattice spacing, $8 \rightarrow 12$, is

definitely outside of the a^2 scaling region and can not be used for continuum extrapolation. Thus we do not discuss these coarse lattices any further. The results are shown in the left panel of figure 1 with the choice of $c = 0.3$. (Note that as a cross check we repeated the calculations with the scale change $s = 2$ and with 3 lattice spacings, corresponding to $8 \rightarrow 16$, $12 \rightarrow 24$ and $18 \rightarrow 36$. All the findings are similar to those obtained with $s = 3/2$.)

For the $s = 3/2$ case with 3 lattice spacings and volume changes $12 \rightarrow 18$, $16 \rightarrow 24$ and $24 \rightarrow 36$ the results can be continuum extrapolated assuming a fit linear in a^2/L^2; see the right panel of figure 1 and figure 2.

5. Conclusions

In this work a running coupling scheme was investigated where the running scale μ is given by the linear size of the system $\mu = 1/L$. The main idea is to use the Yang-Mills gradient flow [1, 2, 3] but to adapt it to a finite volume setting [7]. In principle the original infinite volume construction can also be used to define a scheme where the running is via $\mu = 1/\sqrt{8t}$ where t is the flow time, however in this setup one would need to ensure that finite volume effects are fully under control. In contrast, incorporating finite volume dependence explicitly into the setup eliminates this problem. In addition, a small finite physical volume with appropriate boundary conditions for the fermions guarantees a gap in the spectrum even in the massless case.

Our goal was to determine $g^2(sL)$ as a function of $g^2(L)$ at various lattice spacings. To that end we measured the renormalized coupling $g^2(L)$ and $g^2(sL)$ with the same set of bare couplings, $m = 0$ and β. In the next step we performed an extrapolation to the continuum limit, $a^2/L^2 \rightarrow 0$, for the discrete β-function.

For our main results we used simulations at 3 lattice spacings with $s = 3/2$ and $c = 0.3$. Renormalized couplings between 0 and 2.0 were studied and a controlled continuum extrapolation was carried out. For small renormalized coupling the universal continuum 1-loop result is reproduced and the $\overline{\text{MS}}$ 2-loop result is also consistent with our numerical results; see figure 2. This suggests that for our choice of $s = 3/2$ and $c = 0.3$ the coefficient a_1 connecting the gradient flow scheme to the $\overline{\text{MS}}$ scheme $g_c^2 = g_{\overline{\text{MS}}}^2(1 + a_1(c)g_{\overline{\text{MS}}} + \dots)$ is probably small.

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